A new quantum lower bound method, with an application to strong direct product theorem for quantum search

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Abstract

We present a new method for proving lower bounds on quantum query algorithms. The new method is an extension of adversary method, by analyzing the eigenspace structure of the problem.

Using the new method, we prove a strong direct product theorem for quantum search. This result was previously proven by Klauck, Špalek and de Wolf (quant-ph/0402123) using polynomials method. No proof using adversary method was known before.

1 Introduction

Many quantum algorithms (for example, Grover's algorithm [11] and quantum counting [9]) can be analyzed in the query model where the input is accessed via a black box that answers queries about the values of input bits.

There are two main methods for proving lower bounds on query algorithms: adversary method [3] and polynomials method [7] and both of them have been studied in detail. The limits of adversary method are particularly well understood. The original adversary method [3] has been generalized in several different ways [4, 15, 6]. Špalek and Szegedy [19] then showed that all the generalizations are equivalent and, for certain problems, cannot improve the best known lower bounds. For example [19, 20], the adversary methods of [4, 15, 6] cannot prove a lower bound on a total Boolean function that exceeds $O(\sqrt{C_0(f)C_1(f)})$, where $C_0(f)$ and $C_1(f)$ are the certificate complexities of f on 0-inputs and 1-inputs. This implies that the adversary methods of [4, 15, 6] cannot prove a tight lower bound for element distinctness or improve the best known lower bound for triangle finding. (The complexity of element distinctness is $\Theta(N^{2/3})$

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[2, 5] but the adversary method cannot prove a bound better than $\Omega(\sqrt{N})$. For triangle finding [17], the best known lower bound is $\Omega(N)$ and it is known that it cannot be improved using the adversary method. It is, however, possible that the bound is not tight, because the best algorithm uses $O(N^{1.3})$ queries.)

In this paper, we describe a new version of quantum adversary method which may not be subject to those limitations. We then use the new method to prove a strong direct product theorem for the *K-fold search* problem.

In the K-fold search problem, a black box contains $x_1, \ldots, x_N$ such that $|\{i : x_i = 1\}| = K$ and we have to find all K values $i : x_i = 1$. This problem can be solved with $O(\sqrt{NK})$ queries. It can be easily shown, using any of the previously known methods, that $\Omega(\sqrt{NK})$ queries are required. A more difficult problem is to show that $\Omega(\sqrt{NK})$ queries are required, even if the algorithm only has to be correct with an exponentially small probability c^{-K}, $c > 1$. This result is known as the *strong direct product theorem* for k-fold search. Besides being interesting on its own, the strong direct product theorem is useful for proving time-space tradeoffs for quantum sorting [13] and lower bounds on quantum computers that use advice [1].

The strong direct product theorem for quantum search was first shown by Klauck et al. [13], using polynomials method. No proof using adversary method has been known and, as we show in section 3, the previously known adversary methods are insufficient to prove a strong direct product theorem for K-fold search.

2 Preliminaries

We consider the following problem.

Search for K marked elements, $SEARCH_K(N)$. Given a black box containing $x_1, \ldots, x_N \in \{0, 1\}$ such that $x_i = 1$ for exactly K values $i \in \{1, 2, \ldots, N\}$, find all K values $i_1, \ldots, i_K$ satisfying $x_{i_j} = 1$.

This problem can be viewed as computing an $\binom{N}{K}$-valued function $f(x_1, \ldots, x_N)$ of variables $x_1, \ldots, x_N \in \{0, 1\}$, with values of the function being indices for $\binom{N}{K}$ sets $S \subseteq [N]$ of size K, in some canonical ordering of those sets.

We study this problem in the quantum query model (for a survey on query model, see [10]). In this model, the input bits can be accessed by queries to an oracle X and the complexity of f is the number of queries needed to compute f. A quantum computation with T queries is just a sequence of unitary transformations

$$U_0 \to O \to U_1 \to O \to \ldots \to U_{T-1} \to O \to U_T.$$

The U_j's can be arbitrary unitary transformations that do not depend on the input bits $x_1, \ldots, x_N$. The O's are query (oracle) transformations which depend on $x_1, \ldots, x_N$. To define O, we represent basis states as $|i, z\rangle$ where i consists of $\lceil \log(N+1) \rceil$ bits and z consists of all other bits. Then, O_x maps $|0, z\rangle$ to itself and $|i, z\rangle$ to $(-1)^{x_i}|i, z\rangle$ for $i \in \{1, ..., N\}$ (i.e., we change phase depending on x_i, unless $i = 0$ in which case we do nothing).

The computation starts with a state $|0\rangle$. Then, we apply U_0, O_x, ..., O_x, U_T and measure the final state. The result of the computation are $\lceil \log_2 \binom{N}{K} \rceil$ rightmost bits of

the state obtained by the measurement,which are interpreted as a description for one of $\binom{N}{K}$ subsets $S \subseteq \{1,\ldots,N\}$, $|S| = K$.

3 Overview of adversary method

We describe the adversary method of [3].

Let S be a subset of the set of possible inputs $\{0,1\}^N$. We run the algorithm on a superposition of inputs in S. More formally, let $\mathcal{H}_A$ be the workspace of the algorithm. We consider a bipartite system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_I$ where $\mathcal{H}_I$ is an "input subspace" spanned by basis vectors $|x\rangle$ corresponding to inputs $x \in S$.

Let $U_T O U_{T-1} \ldots U_0$ be the sequence of unitary transformations on $\mathcal{H}_A$ performed by the algorithm A (with $U_0,\ldots,U_T$ being the transformations that do not depend on the input and O being the query transformations). We transform it into a sequence of unitary transformations on $\mathcal{H}$. A unitary transformation U_i on $\mathcal{H}_A$ corresponds to the transformation $U_i' = U_i \otimes I$ on the whole $\mathcal{H}$. The query transformation O corresponds to a transformation O' that is equal to O_x on subspace $H_A \otimes |x\rangle$.

We perform the sequence of transformations $U_T' O' U_{T-1}' \ldots U_0'$ on the starting state

$$|\psi_{start}\rangle = |0\rangle \otimes \sum_{x \in S} \alpha_x |x\rangle.$$

Then, the final state is

$$|\psi_{end}\rangle = \sum_{x \in S} \alpha_x |\psi_x\rangle \otimes |x\rangle$$

where $|\psi_x\rangle$ is the final state of $A = U_T O U_{T-1} \ldots U_0$ on the input x. This follows from the fact that the restrictions of $U_T', O', U_{T-1}', \ldots, U_0'$ to $\mathcal{H}_A \otimes |x\rangle$ are U_T, O_x, U_{T-1}, …, U_0 and these are exactly the transformations of the algorithm A on the input x.

Let ρ_{end} be the reduced density matrix of the $\mathcal{H}_I$ register of the state $|\psi_{end}\rangle$. The adversary method of [3, 4] works by showing the following two statements

- Let $x \in S$ and $y \in S$ be such that $f(x) \neq f(y)$ (where f is the function that is being computed). If the algorithm outputs the correct answer with probability $1-\epsilon$ on both x and y, then $|\rho_{end})_{x,y}| \leq 2\sqrt{\epsilon(1-\epsilon)}|\alpha_x||\alpha_y|$.
- for any algorithm that uses T queries, there are inputs $x, y \in S$ such that $(\rho_{end})_{x,y} > 2\sqrt{\epsilon(1-\epsilon)}|\alpha_x||\alpha_y|$ and $f(x) \neq f(y)$.

These two statements together imply that any algorithm computing f must use more than T queries.

An equivalent approach [12, 4] is to consider the inner products $\langle\psi_x|\psi_y\rangle$ between the final states $|\psi_x\rangle$ and $|\psi_y\rangle$ of the algorithm on inputs x and y. Then, $|(\rho_{end})_{x,y}| \leq 2\sqrt{\epsilon(1-\epsilon)}|\alpha_x||\alpha_y|$ is equivalent to $|\langle\psi_x|\psi_y\rangle| \leq 2\sqrt{\epsilon(1-\epsilon)}$.

As a result, both of the above statements can be described in terms of inner products $\langle\psi_x|\psi_y\rangle$, without explicitly introducing the register $\mathcal{H}_I$. The first statement says that, for the algorithm to succeed on inputs x, y such that $f(x) \neq f(y)$, the states $|\psi_x\rangle$ and $|\psi_y\rangle$ must be sufficiently far apart one from another (so that the inner product

$|\langle\psi_x|\psi_y\rangle|$ is at most $2\sqrt{\epsilon(1-\epsilon)}$). The second statement says that this is impossible if the algorithm only uses T queries.

This approach breaks down if we consider computing a function f with success probability $p < 1/2$. (f has to have more than 2 values for this task to be nontrivial.) Then, $|\psi_x\rangle$ and $|\psi_y\rangle$ could be the same and the algorithm may still succeed on both inputs, if it outputs x with probability 1/2 and y with probability 1/2. In the case of strong direct product theorems, the situation is even more difficult. Since the algorithm only has to be correct with a probability c^{-K}, the algorithm could have almost the same final state on c^K different inputs and still succeed on every one of them.

In this paper, we present a new method that does not suffer from this problem. Our method, described in the next section, uses the idea of augmenting the algorithm with an input register $\mathcal{H}_I$, together with two new ingredients:

1. **Symmetrization.** We symmetrize the algorithm by applying a random permutation $\pi \in S_N$ to the input $x_1, \ldots, x_N$.
2. **Eigenspace analysis.** We study the eigenspaces of ρ_{start}, ρ_{end} and density matrices describing the state of $\mathcal{H}_I$ at intermediate steps and use them to bound the progress of the algorithm.

The eigenspace analysis is the main new technique. Symmetrization is necessary to simplify the structure of the eigenspaces, to make the eigenspace analysis possible.

4 Our result

Theorem 1 *There exist ϵ and c satisfying $\epsilon > 0$, $0 < c < 1$ such that, for any $K \leq N/2$, solving $SEARCH_K(N)$ with probability at least c^K requires $(\epsilon - o(1))\sqrt{NK}$ queries.*

Proof: Let $\mathcal{A}$ be an algorithm for $SEARCH_K(N)$ that uses $T \leq \epsilon\sqrt{NK}$ queries.

We first "symmetrize" $\mathcal{A}$ by adding an extra register $\mathcal{H}_P$ holding a permutation $\pi \in S_N$. Initially, $\mathcal{H}_P$ holds a uniform superposition of all permutations π: $\frac{1}{\sqrt{N!}}\sum_{\pi\in S_N}|\pi\rangle$. Before each query O, we insert a transformation $|i\rangle|\pi\rangle \rightarrow |\pi^{-1}(i)\rangle|\pi\rangle$ on the part of the state containing the index i to be queried and $\mathcal{H}_P$. After the query, we insert a transformation $|i\rangle|\pi\rangle \rightarrow |\pi(i)\rangle|\pi\rangle$. At the end of algorithm, we apply the transformation $|i_1\rangle \ldots |i_K\rangle|\pi\rangle \rightarrow |\pi^{-1}(i_1)\rangle \ldots |\pi^{-1}(i_K\rangle|\pi\rangle$. The effect of the symmetrization is that, on the subspace $|s\rangle \otimes |\pi\rangle$, the algorithm is effectively running on the input x_1, ..., x_N with $x_{\pi(i_1)} = \ldots = x_{\pi(i_K)} = 1$.

If the original algorithm $\mathcal{A}$ succeeds on every input $(x_1, \ldots, x_N)$ with probability at least ϵ, the symmetrized algorithm also succeeds with probability at least ϵ, since its success probability is just the average of the success probabilities of $\mathcal{A}$ over all $(x_1, \ldots, x_N)$ with exactly K values $x_i = 1$. Next, we recast $\mathcal{A}$ into a different form, using a register that stores the input $x_1, \ldots, x_N$, as in section 3.

Let $\mathcal{H}_A$ be the Hilbert space on which the symmetrized version of $\mathcal{A}$ operates. Let $\mathcal{H}_I$ be an $\binom{N}{K}$-dimensional Hilbert space whose basis states correspond to inputs $(x_1, \ldots, x_N)$ with exactly K values $i : x_i = 1$. We transform $\mathcal{A}$ into a sequence of transformations on a Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_I$. A non-query transformation U on

$\mathcal{H}_A$ is replaced with $U \otimes I$ on $\mathcal{H}$. A query is replaced by a transformation O that is equal to $O_{x_1,\ldots,x_N} \otimes I$ on the subspace consisting of states of the form $|s\rangle_A \otimes |x_1 \ldots x_N\rangle_I$. The starting state of the algorithm on Hilbert space $\mathcal{H}$ is $|\varphi_0\rangle = |\psi_{start}\rangle_A \otimes |\psi_0\rangle_I$ where $|\psi_{start}\rangle$ is the starting state of $\mathcal{A}$ as an algorithm acting on $\mathcal{H}_A$ and $|\psi_0\rangle$ is the uniform superposition of all basis states of $\mathcal{H}_I$:

$$|\psi_0\rangle = \frac{1}{\sqrt{\binom{N}{K}}} \sum_{x_1,\ldots,x_N : x_1+\ldots+x_N=K} |x_1 \ldots x_N\rangle.$$

Let $|\psi_t\rangle$ be the state of the algorithm $\mathcal{A}$, as a sequence of transformations on $\mathcal{H}$, after the t^{th} query. Let ρ_t be the mixed state obtained from $|\psi_t\rangle$ by tracing out the $\mathcal{H}_A$ register.

We claim that the states ρ_t have a special form, due to our symmetrization step.

Lemma 2 *The entries $(\rho_t)_{x,y}$ are the same for all $x = (x_1, \ldots, x_N)$, $y = (y_1, \ldots, y_N)$ with the same cardinality of the set $\{l : x_l = y_l = 1\}$.*

Proof: Since ρ_t is independent of the way how the $\mathcal{H}_A \otimes \mathcal{H}_S$ is traced out, we first measure $\mathcal{H}_S$ (in the $|\pi\rangle$ basis) and then measure $\mathcal{H}_A$ (arbitrarily). When measuring $\mathcal{H}_S$, every π is obtained with an equal probability. Let $\rho_{t,\pi}$ be the reduced density matrix of $\mathcal{H}_I$, conditioned on the measurement of $\mathcal{H}_S$ giving π. Then,

$$\rho_t = \sum_{\pi} \frac{1}{N!} \rho_{t,\pi}.$$

The entry $(\rho_{t,\pi})_{x,y}$ is the same as the entry $(\rho_{t,id})_{\pi^{-1}(x),\pi^{-1}(y)}$ because the symmetrization by π maps $\pi^{-1}(x), \pi^{-1}(y)$ to x, y. For every x, y, x', y' with $|\{i : x_i = y_i = 1\}| = |\{i : x'_i = y'_i = 1\}|$, there is an equal number of permutations π mapping $\pi(x) = x'$, $\pi(y) = y'$. Therefore, $(\rho_t)_{x,y}$ is the average of $(\rho_{t,id})_{x',y'}$ over all x', y' with $|\{l : x_l = y_l = 1\}| = |\{l : x'_l = y'_l = 1\}|$. This means that $(\rho_t)_{x,y}$ only depends on $|\{l : x_l = y_l = 1\}|$. ■

Any $\binom{N}{K} \times \binom{N}{K}$ matrix with this property shares the same eigenspaces. Namely [14], its eigenspaces are S_0, S_1, ..., S_K where $T_0 = S_0$ consists of multiples of $|\psi_0\rangle$ and, for $j > 0$, $S_j = T_j - T_{j-1}$, with T_j being the space spanned by all states

$$|\psi_{i_1,\ldots,i_j}\rangle = \frac{1}{\sqrt{\binom{N}{K-j}}} \sum_{\substack{x_1,\ldots,x_N: \\ x_1+\ldots+x_N=K, \\ x_{i_1}=\ldots=x_{i_j}=1}} |x_1 \ldots x_N\rangle.$$

Let τ_j be the completely mixed state over the subspace S_j.

Lemma 3 *There exist $p_{t,0} \geq 0$, ..., $p_{t,K} \geq 0$ such that $\rho_t = \sum_{j=0}^{K} p_{t,j} \tau_j$.*

Proof: According to [14], S_0, ..., S_K are the eigenspaces of ρ_t. Therefore, ρ_t is a linear combination of the projectors to S_0, ..., S_K. Since τ_j is a multiple of the projector to

S_j, we have

$$\rho_t = \sum_{j=0}^{K} p_{t,j}\tau_j.$$

Since ρ_t is a density matrix, it must be positive semidefinite. This means that $p_{t,0} \geq 0$, ..., $p_{t,K} \geq 0$. ■

Let $q_{t,j} = p_{t,j} + p_{t,j+1} + \ldots + p_{t,K}$. The theorem now follows from the following lemmas.

Lemma 4 *$p_{0,0} = 1$, $p_{0,j} = 0$ for $j > 0$.*

Proof: The state $|\varphi_0\rangle$ is just $|\psi_{start}\rangle \otimes |\psi_0\rangle$. Tracing out $|\psi_{start}\rangle$ leaves the state $\rho_0 = |\psi_0\rangle\langle\psi_0|$. ■

Lemma 5 *For all $j \in \{1, \ldots, K\}$ and all t, $q_{t+1,j+1} \leq q_{t,j+1} + \frac{4\sqrt{K}}{\sqrt{N}} q_{t,j}$*

Proof: In section 5. ■

Lemma 6 $q_{t,j} \leq \binom{t}{j} \left(\frac{4\sqrt{K}}{\sqrt{N}}\right)^j$.

Proof: By induction on t. The base case, $t = 0$ follows immediately from $p_{0,0} = 1$ and $p_{0,1} = \ldots = p_{0,K} = 0$. For the inductive case, we have

$$q_{t+1,j} \leq q_{t,j} + \frac{4\sqrt{K}}{\sqrt{N}} q_{t,j-1} \leq \binom{t}{j} \left(\frac{4\sqrt{K}}{\sqrt{N}}\right)^j + \frac{4\sqrt{K}}{\sqrt{N}} \binom{t}{j-1} \left(\frac{4\sqrt{K}}{\sqrt{N}}\right)^{j-1}$$

$$\leq \left(\binom{t}{j} + \binom{t}{j-1}\right) \left(\frac{4\sqrt{K}}{\sqrt{N}}\right)^j = \binom{t+1}{j} \left(\frac{4\sqrt{K}}{\sqrt{N}}\right)^j,$$

with the first inequality following from Lemma 5 and the second inequality following from the inductive assumption. ■

Lemma 7 *If $t \leq 0.03\sqrt{NK}$, then $p_{t,j} < 0.65^j$ for all $j > K/2$.*

Proof: We have

$$q_{t,j} \leq \binom{t}{j} \left(\frac{4\sqrt{K}}{\sqrt{N}}\right)^j < \frac{t^j}{j!} \left(\frac{4\sqrt{K}}{\sqrt{N}}\right)^j$$

$$\leq \frac{t^j e^j}{j^j} \left(\frac{4\sqrt{K}}{\sqrt{N}}\right)^j = \left(\frac{4\sqrt{K} et}{\sqrt{N} j}\right)^j,$$

where the third inequality follows from $j! \geq (\frac{j}{e})^j$ which is a consequence of the Stirling's formula. Let $j > K/2$ and $t \leq 0.03\sqrt{NK}$. Then,

$$\frac{4\sqrt{K} et}{\sqrt{N} j} \leq \frac{0.12 e \sqrt{K}\sqrt{NK}}{\sqrt{N} K/2} < 0.65,$$

implying the lemma. ■

Lemma 8 *The success probability of $\mathcal{A}$ is at most*

$$\frac{\binom{N}{K/2}}{\binom{N}{K}} + 4\sqrt{\sum_{j=K/2+1}^{K} p_{T,j}}.$$

Proof: In section 6. ■

To complete the proof, given the two Lemmas, we choose a constant $c > \sqrt[4]{0.65} = 0.8979...$ and set $\epsilon = 0.04$. Then, by Lemma 8, the success probability of $\mathcal{A}$ is at most

$$\frac{\binom{N}{K/2}}{\binom{N}{K}} + 4\sqrt{\frac{K}{2}0.65^{K/2}}.$$

The first term is equal to

$$\frac{\binom{N}{K/2}}{\binom{N}{K}} = \frac{K!(N-K)!}{(K/2)!(N-K/2)!} \leq \frac{K!}{(K/2)!(N-K)^{K/2}}$$

$$= O\left(\frac{(K/e)^K}{(K/2e)^{K/2}(N-K)^{K/2}}\right) = O\left(\left(\frac{2K}{e(N-K)}\right)^{K/2}\right)$$

$$= O\left(\left(\frac{2}{e}\right)^{K/2}\right) = O(0.857...^K),$$

with the third step following from Stirling's approximation and the fifth step following from $K < N/2$. The second part, $\sqrt{\frac{K}{2}0.65^{K/2}}$ is less than $c^K/2$ if K is sufficiently large.

It remains to prove the two lemmas.

5 Proof of Lemma 5

We decompose the state $|\psi_t\rangle$ as $\sum_{i=0}^{N} a_i|\psi_{t,i}\rangle$, with $|\psi_{t,i}\rangle$ being the part in which the query register contains $|i\rangle$. Because of symmetrization, we must have $|a_1| = |a_2| = \ldots = |a_N|$. Let $\rho_{t,i} = |\psi_{t,i}\rangle\langle\psi_{t,i}|$. Then,

$$\rho_t = \sum_{i=0}^{N} a_i^2 \rho_{t,i}. \tag{1}$$

For $i > 0$, we have

Claim 9 *Let $i \in \{1,\ldots,N\}$. The entry $(\rho_{t,i})_{x,y}$ only depends on x_i, y_i and the cardinality of $\{l : l \neq i, x_l = y_l = 1\}$.*

Proof: Similar to lemma 2. ■

We now describe the eigenspaces of matrices $\rho_{t,i}$. The proofs of some claims are postponed to section 7.

We define the following subspaces of states. Let $T_j^{i,0}$ be the subspace spanned by all states

$$|\psi^{i,0}_{i_1,\ldots,i_j}\rangle = \frac{1}{\sqrt{\binom{N-j-1}{K-j}}} \sum_{\substack{x:|x|=K \\ x_{i_1}=\ldots=x_{i_j}=1, x_i=0}} |x_1 \ldots x_N\rangle$$

and $T_j^{i,1}$ be the subspace spanned by all states

$$|\psi^{i,1}_{i_1,\ldots,i_j}\rangle = \frac{1}{\sqrt{\binom{N-j-1}{K-j-1}}} \sum_{\substack{x:|x|=K \\ x_{i_1}=\ldots=x_{i_j}=1, x_i=1}} |x_1 \ldots x_N\rangle.$$

Let $S_j^{i,0} = T_j^{i,0} \cap (T_{j-1}^{i,0})^\perp$ and $S_j^{i,1} = T_j^{i,1} \cap (T_{j-1}^{i,1})^\perp$. Equivalently, we can define $S_j^{i,0}$ and $S_j^{i,1}$ as the subspaces spanned by the states $|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$ and $|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$, respectively, with

$$|\tilde{\psi}^{i,l}_{i_1,\ldots,i_j}\rangle = P_{(T^{i,l}_{j-1})^\perp} |\psi^{i,l}_{i_1,\ldots,i_j}\rangle.$$

Let $S^i_{\alpha,\beta,j}$ be the subspace spanned by all states

$$\alpha \frac{|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle}{\||\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle\|} + \beta \frac{|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle}{\||\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle\|}. \tag{2}$$

Claim 10 *Every eigenspace of $\rho_{t,i}$ is a direct sum of subspaces $S^i_{\alpha,\beta,j}$ for some α, β, j.*

Proof: In section 7. ■

Let $\tau^i_{\alpha,\beta,j}$ be the completely mixed state over $S^i_{\alpha,\beta,j}$. Similarly to lemma 3, we can write $\rho_{t,i}$ as

$$\rho_{t,i} = \sum_{(\alpha,\beta,j)\in A_{t,i}} p^i_{\alpha,\beta,j} \tau^i_{\alpha,\beta,j}, \tag{3}$$

where (α,β,j) range over some finite set $A_{t,i}$. (This set is finite because the $\mathcal{H}_I$ register holding $|x_1 \ldots x_N\rangle$ is finite dimensional and, therefore, decomposes into a direct sum of finitely many eigenspaces.) For every pair $(\alpha,\beta,j) \in A_{t,i}$, we normalize α,β by multiplying them by the same constant so that $\alpha^2+\beta^2=1$. Querying x_i transforms this state to

$$\rho'_{t,i} = \sum_{(\alpha,\beta,j)\in A_{t,i}} p^i_{\alpha,\beta,j} \tau^i_{\alpha,-\beta,j},$$

because $|\tilde{\psi}^{i,l}_{i_1,\ldots,i_j}\rangle$ is a superposition of $|x\rangle$ with $x_i = l$ and, therefore, a query leaves $|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$ unchanged and flips a phase on $|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$. If $i=0$, we have $\rho'_{t,0} = \rho_{t,0}$, because, if the query register contains $|0\rangle$, the query maps any state to itself, thus leaving $\rho_{t,0}$ unchanged.

Claim 11 *Let* $\alpha_0 = \sqrt{\frac{N-K}{N-j}}\|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\|$ *and* $\beta_0 = \sqrt{\frac{K-j}{N-j}}\|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\|$.

(i) $S^i_{\alpha_0,\beta_0,j} \subseteq S_j$;

(ii) $S^i_{\beta_0,-\alpha_0,j} \subseteq S_{j+1}$.

Proof: In section 7. ■

Corollary 12 *For any* α, β, $S^i_{\alpha,\beta,j} \subseteq S_j \cup S_{j+1}$.

Proof: We have $S_{\alpha,\beta,j} \subseteq S^{i,0}_j \cup S^{i,1}_j$, since $S_{\alpha,\beta,j}$ is spanned by linear combinations of states $|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$ (which belong to $S^{i,0}_j$) and states $|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$ (which belong to $S^{i,1}_j$). As shown in the proof of claim 11 above,

$$S^{i,0}_j \cup S^{i,1}_j \subseteq S_{\alpha_0,\beta_0,j} \cup S_{-\beta_0,\alpha_0,j} \subseteq S_j \cup S_{j+1}.$$

■

The next claim quantifies the overlap between $S^i_{\alpha,\beta,j}$ and S_{j+1}.

Claim 13

$$TrP_{S_{j+1}}\tau^i_{\alpha,\beta,j} = \frac{|\alpha\beta_0 - \beta\alpha_0|^2}{\alpha_0^2 + \beta_0^2}$$

Proof: In section 7. ■

To be able to use this bound, we also need to bound α_0 and β_0.

Claim 14 $\frac{\beta_0}{\sqrt{\alpha_0^2+\beta_0^2}} \leq \sqrt{\frac{4(K-j)}{N+3K-4j}}$.

Proof: In section 7. ■

We can now complete the proof of lemma 5. By projecting both sides of $\rho_t = \sum_i p_{t,i}\tau_i$ to $(T_j)^\perp = S_{j+1} \cup \ldots S_K$ and taking trace, we get

$$TrP_{(T_j)^\perp}\rho_t = \sum_{j'=0}^{K} p_{t,j} TrP_{(T^j)^\perp}\tau_{j'} = \sum_{j'=j}^{K} p_{t,j} = q_{t,j}, \tag{4}$$

with the second equality following because the states $\tau_{j'}$ are uniform mixtures over subspaces $S_{j'}$ and $S_0, \ldots, S_j$ are contained in T_j while $S_{j+1}, \ldots, S_K$ are contained in $(T_j)^\perp$. Because of equations (1), (**??**) and (3), this means that

$$q_{t,j+1} = a_0^2 TrP_{(T_j)^\perp}\rho_{t,0} + \sum_{i=1}^{N} a_i^2 \sum_{(\alpha,\beta,j')\in A_{t,i}} p^i_{\alpha,\beta,j'} TrP_{(T_j)^\perp}\tau^i_{\alpha,\beta,j'}. \tag{5}$$

Decomposing the state after the query in a similar way, we get

$$q_{t+1,j+1} = a_0^2 TrP_{(T_j)^\perp}\rho'_{t,0} + \sum_{i=1}^{N} a_i^2 \sum_{(\alpha,\beta,j')\in A_{t,i}} p^i_{\alpha,\beta,j'} TrP_{(T_j)^\perp}\tau^i_{\alpha,-\beta,j'}.$$

By substracting the two sums and using $\rho'_{t,0} = \rho_{t,0}$, we get

$$q_{t+1,j+1} - q_{t,j+1} = \sum_{i=1}^{N} a_i^2 \sum_{(\alpha,\beta,j') \in A_{t,i}} p^i_{\alpha,\beta,j'} TrP_{(T_j)^\perp}(\tau^i_{\alpha,-\beta,j'} - \tau^i_{\alpha,\beta,j'}). \tag{6}$$

We now claim that all the terms in this sum with $j' \neq j$ are 0. For $j' < j$, $S_{\alpha,\beta,j'} \subseteq T_{j'+1} \subseteq T_j$, implying that $TrP_{(T_j)^\perp}\tau^i_{\alpha,\beta,j'} = 0$ and, similarly, $TrP_{(T_j)^\perp}\tau^i_{\alpha,-\beta,j'} = 0$. For $j' > j$, $S_{\alpha,\beta,j'} \subseteq S_{j'} \cup S_{j'+1} \subseteq (T_j)^\perp$, implying that

$$TrP_{(T_j)^\perp}\tau^i_{\alpha,\beta,j'} = 1, \quad TrP_{(T_j)^\perp}\tau^i_{\alpha,-\beta,j'} = 1$$

and the difference of the two is 0. By removing those terms from (6), we get

$$q_{t+1,j+1} - q_{t,j+1} = \sum_{i=1}^{N} a_i^2 \sum_{(\alpha,\beta,j) \in A_{t,i}} p^i_{\alpha,\beta,j} TrP_{(T_j)^\perp}(\tau^i_{\alpha,-\beta,j} - \tau^i_{\alpha,\beta,j}). \tag{7}$$

We have

$$TrP_{(T_j)^\perp}(\tau^i_{\alpha,-\beta,j} - \tau^i_{\alpha,\beta,j}) = TrP_{S_{j+1}}(\tau^i_{\alpha,-\beta,j} - \tau^i_{\alpha,\beta,j})$$
$$= \frac{|\alpha\beta_0 + \beta\alpha_0|^2}{\alpha_0^2 + \beta_0^2} - \frac{|\alpha\beta_0 - \beta\alpha_0|^2}{\alpha_0^2 + \beta_0^2},$$

with the first equality following from Corollary 12, $S_j \subseteq T_j$ and $S_{j+1} \subseteq (T_j)^\perp$ and the second equality following from Claim 13. This is at most

$$4\frac{|\alpha\beta\alpha_0\beta_0|}{\alpha_0^2 + \beta_0^2} \leq 2\frac{\alpha_0\beta_0}{\alpha_0^2 + \beta_0^2}$$

$$= 2\frac{\alpha_0}{\sqrt{\alpha_0^2 + \beta_0^2}} \frac{\beta_0}{\sqrt{\alpha_0^2 + \beta_0^2}} \leq 2\sqrt{\frac{4(K-j)}{N + 3K - 4j}} \leq 2\sqrt{\frac{4K}{N}},$$

with the first inequality following from $|\alpha\beta| \leq \frac{|\alpha|^2 + |\beta|^2}{2} = \frac{1}{2}$ and the second inequality following from Claim 14 and $\frac{\alpha_0}{\sqrt{\alpha_0^2+\beta_0^2}} \leq 1$. Together with equation (6), this means

$$q_{t+1,j+1} - q_{t,j+1} \leq \frac{4\sqrt{K}}{\sqrt{N}} \sum_{i=1}^{N} a_i^2 \sum_{(\alpha,\beta,j) \in A_{t,i}} p^i_{\alpha,\beta,j} \tag{8}$$

Similarly to equation (4) we have

$$p_{t,j+1} + p_{t,j} = TrP_{(S_j \cup S_{j+1})}\rho_t.$$

We can then express the right hand side similarly to equation (5), as a sum of terms $p^0_{j'} TrP_{(S_j \cup S_{j+1})}\tau_{j'}$ and $p^i_{\alpha,\beta,j'} TrP_{(S_j \cup S_{j+1})}\tau^i_{\alpha,\beta,j'}$. Since $S^i_{\alpha,\beta,j} \subseteq S_j \cup S_{j+1}$ (by corollary 12), we have $TrP_{(S_j \cup S_{j+1})}\tau^i_{\alpha,\beta,j} = 1$. This means that

$$p_{t,j+1} + p_{t,j} \geq \sum_{i=1}^{N} a_i^2 \sum_{(\alpha,\beta,j) \in A_{t,i}} p^i_{\alpha,\beta,j}.$$

Together with equation (8), this implies

$$q_{t+1,j+1} - q_{t,j+1} \leq \frac{4\sqrt{K}}{\sqrt{N}}(p_{t,j} + p_{t,j+1}) \leq \frac{4\sqrt{K}}{\sqrt{N}} \sum_{j'=j}^{K} p_{t,j'} = \frac{4\sqrt{K}}{\sqrt{N}} q_{t,j}.$$

■

6 Proof of Lemma 8

We start with the case, when $p_{T,K/2+1} = \ldots = p_{T,K} = 0$.

Lemma 15 *If $p_{T,K/2+1} = \ldots = p_{T,K} = 0$, the success probability of $\mathcal{A}$ is at most $\frac{\binom{N}{K/2}}{\binom{N}{K}}$.*

Proof: Let $|\psi\rangle$ be the final state. The state of $\mathcal{H}_I$ register lies in $T_{K/2}$, which is a $\binom{N}{K/2}$ dimensional space. Therefore, there is a Schmidt decomposition for $|\psi\rangle$ with at most $\binom{N}{K/2}$ terms. This means that the state of $\mathcal{H}_A$ lies in a $\binom{N}{K/2}$ subspace of $\mathcal{H}_A \otimes H_S$.

We express the final state as

$$|\psi\rangle = \sum_{x:|x|=K} \frac{1}{\sqrt{\binom{N}{K}}} |\psi_x\rangle |x\rangle.$$

We can think of $|\psi_x\rangle$ as a quantum encoding for x and the final measurement as a decoding procedure that takes $|\psi_x\rangle$ and produces a guess for x. The probability that algorithm $\mathcal{A}$ succeeds is then equal to the average success probability of the encoding. We now use

Theorem 16 *[18] For any encoding $|\psi_x\rangle$ of M classical values in by quantum states in d dimensions, the probability of success is at most $\frac{d}{M}$.*

In our case, $M = \binom{N}{K}$ and $d = \binom{N}{K/2}$ because the states $|\psi\rangle$ all lie in a $\binom{N}{K/2}$-dimensional subspace of $\mathcal{H}_A \otimes \mathcal{H}_S$. Therefore, Theorem 16 implies Lemma 15. ■

We decompose the state $|\psi_T\rangle$ as $\sqrt{1-\delta}|\psi'_T\rangle + \sqrt{\delta}|\psi''_T\rangle$ where $|\psi'_T\rangle$ is in the subspace $\mathcal{H}_A \otimes \cup_{j=0}^{K/2} S_j$ and $|\psi''_T\rangle$ is in $\mathcal{H}_A \otimes \cup_{j=K/2+1}^{K} S_j$. We have

$$\delta = \sum_{j=K/2+1}^{K} p_{T,j}.$$

The success probability of $\mathcal{A}$ is the probability that, if we measure both the register of $\mathcal{H}_A$ containing the result of the computation and $\mathcal{H}_I$, then, we get $i_1, \ldots, i_K$ and $x_1, \ldots, x_N$ such that $x_{i_1} = \ldots = x_{i_K} = 1$.

Consider the probability of getting $i_1, \ldots, i_K$ and $x_1, \ldots, x_N$ such that $x_{i_1} = \ldots = x_{i_K} = 1$, when measuring $|\psi'_T\rangle$ (instead of $|\psi_T\rangle$). By Lemma 15, this probability is at most $\frac{\binom{N}{K/2}}{\binom{N}{K}}$. We have

$$\|\psi_T - \psi'_T\| \leq (1 - \sqrt{1-\delta^2})\|\psi'_T\| + \sqrt{\delta}\|\psi''_T\| = (1 - \sqrt{1-\delta^2}) + \sqrt{\delta} \leq 2\sqrt{\delta}.$$

We now apply

Lemma 17 *[8] For any states $|\psi\rangle$ and $|\psi'\rangle$ and any measurement M, the variational distance between the probability distributions obtained by applying M to $|\psi\rangle$ and $|\psi'\rangle$ is at most $2\|\psi - \psi'\|$.*

By Lemma 17, the probabilities of getting $i_1, \ldots, i_K$ and $x_1, \ldots, x_N$ such that $x_{i_1} = \ldots = x_{i_K} = 1$, when measuring $|\psi_T\rangle$ and $|\psi'_T\rangle$ differ by at most $4\sqrt{\delta} = 4\sqrt{\sum_{j=K/2+1}^{K} p_{T,j}}$. Therefore, the success probability of $\mathcal{A}$ is at most

$$\frac{\binom{N}{K/2}}{\binom{N}{K}} + 4\sqrt{\sum_{j=K/2+1}^{K} p_{T,j}}.$$

7 Structure of the eigenspaces of $\rho_{t,i}$

In this section, we prove claims 10, 11, 13 and 14 describing the structure of the eigenspaces of $\rho_{t,i}$.

Proof: [of Claim 10] We rearrange the rows and the columns of $\rho_{t,i}$ so that all rows and columns corresponding to $|x_1 \ldots x_N\rangle$ with $x_i = 0$ are before the rows and the columns corresponding to $|x_1 \ldots x_N\rangle$ with $x_i = 1$. We then express $\rho_{t,i}$ as

$$\rho_{t,i} = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

with A being a $\binom{N-1}{K} \times \binom{N-1}{K}$ square matrix indexed by $|x_1 \ldots x_N\rangle$ with $x_i = 0$, D being a $\binom{N-1}{K-1} \times \binom{N-1}{K-1}$ square matrix indexed by $|x_1 \ldots x_N\rangle$ with $x_i = 1$ and B and C being rectangular matrices with rows (columns) indexed by $|x_1 \ldots x_N\rangle$ with $x_i = 0$ and columns (rows) indexed by $|x_1 \ldots x_N\rangle$ with $x_i = 1$.

We claim that

$$\rho_{t,i}|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle = a_{11}|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle + a_{12}|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle,$$

$$\rho_{t,i}|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle = a_{21}|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle + a_{22}|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle, \quad (9)$$

where a_{11}, a_{12}, a_{21}, a_{22} are independent of $i_1, \ldots, i_j$. To prove that, we first note that A and D are matrices where A_{xy} and D_{xy} only depends on $|\{t : x_t = y_t\}|$. Therefore, the results of Knuth[14] about eigenspaces of such matrices apply. This means that $S^{i,0}_j$ an $S^{i,1}_j$ are eigenspaces for A and D, respectively, and

$$A|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle = a_{11}|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle,$$

$$D|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle = a_{22}|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle,$$

where a_{11} and a_{22} are the eigenvalues of A and D for the eigenspaces $S^{i,0}_j$ and $S^{i,1}_j$. It remains to prove that

$$B|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle = a_{12}|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle, \quad (10)$$

$$C|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle = a_{21}|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle. \tag{11}$$

Let M be a rectangular matrix, with entries indexed by x, y, with $|x| = |y| = K$ and $x_i = 1$ and $y_i = 0$. The entries of M are $M_{xy} = 1$ if x and y differ in two places, with $x_i = 1$, $y_i = 0$ and $x_l = 0$, $y_l = 1$ for some $l \neq i$ and $M_{xy} = 0$ otherwise. We claim

$$M|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle = c|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle \tag{12}$$

for some c that may depend on N, k and j but not on $i_1, \ldots, i_j$. To prove that, we need to prove two things. First,

$$M|\psi^{i,0}_{i_1,\ldots,i_j}\rangle = c|\psi^{i,1}_{i_1,\ldots,i_j}\rangle. \tag{13}$$

This follows by

$$M|\psi^{i,0}_{i_1,\ldots,i_j}\rangle = \frac{1}{\sqrt{\binom{N-j-1}{k-j}}} \sum_{\substack{x:x_{i_1}=\ldots=x_{i_j}=1,\\ x_i=0}} M|x\rangle$$

$$= \frac{1}{\sqrt{\binom{N-j-1}{K-j}}} \sum_{\substack{x:x_{i_1}=\ldots=x_{i_j}=1\\ x_i=0}} \sum_{l:x_l=1} |x_1 \ldots x_{l-1} 0 x_{l+1} \ldots x_{i-1} 1 x_{i+1} \ldots x_N\rangle$$

$$= \frac{1}{\sqrt{\binom{N-j-1}{K-j}}}(N-K) \sum_{\substack{y:y_{i_1}=\ldots=y_{i_j}=1\\ y_i=1}} |y\rangle = \sqrt{(K-j)(N-K)}|\psi^{i,1}_{i_1,\ldots,i_j}\rangle.$$

Second, $M(T^{i,0}_j) \subseteq T^{i,1}_j$ and $M(T^{i,0}_j)^\perp \subseteq (T^{i,1}_j)^\perp$. The first statement is immediately follows from equation (13), because the subspaces $T^{i,0}_j$, $T^{i,1}_j$ are spanned by the states $|\psi^{i,0}_{i_1,\ldots,i_j}\rangle$ and $|\psi^{i,1}_{i_1,\ldots,i_j}\rangle$, respectively. To prove the second statement, let $|\psi\rangle \in (T^{i,0}_j)^\perp$, $|\psi\rangle = \sum_x a_x|x\rangle$. We would like to prove $M|\psi\rangle \in (T^{i,1}_j)^\perp$. This is equivalent to $\langle\psi^{i,1}_{i_1,\ldots,i_j}|M|\psi\rangle = 0$ for all $i_1, \ldots, i_j$. We have

$$\langle\psi^{i,1}_{i_1,\ldots,i_j}|M|\psi\rangle = \frac{1}{\sqrt{\binom{N-j-1}{K-j-1}}} \sum_{y:y_{i_1}=\ldots=y_{i_j}=1} \langle y|M|\psi\rangle$$

$$= \frac{1}{\sqrt{\binom{N-j-1}{K-j-1}}} \sum_{\substack{x:x_{i_1}=\ldots=x_{i_j}=1,\\ x_i=0}} \sum_{\substack{l:x_l=1,\\ l\notin\{i_1,\ldots,i_j\}}} a_x$$

$$= \frac{1}{\sqrt{\binom{N-j-1}{K-j-1}}}(K-j) \sum_{x:x_{i_1}=\ldots=x_{i_j}=1} a_x = 0.$$

The first equality follows by writing out $\langle\psi^{i,1}_{i_1,\ldots,i_j}|$, the second equality follows by writing out M. The third equality follows because, for every x with $|x| = K$ and $x_{i_1} = \ldots = x_{i_j} = 1$, there are $K - j$ more $l \in [N]$ satisfying $x_l = 1$. The fourth equality follows

because $\sum_{x:x_{i_1}=\ldots=x_{i_j}=1} a_x$ is a constant times $\langle\psi^{i,0}_{i_1,\ldots,i_j}|\psi\rangle$ and $\langle\psi^{i,0}_{i_1,\ldots,i_j}|\psi\rangle = 0$, because $|\psi\rangle \in (T^{i,0}_j)^\perp$.

Furthermore, BM is an $\binom{N-1}{K} \times \binom{N-1}{K}$ matrix, with $(BM)_{x,y}$ only depending on $|\{l : x_l = y_l = 1\}|$. Therefore, $S^{i,1}_j$ is an eigenspace of BM and, since $|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle \in S^{i,1}_j$, we have

$$BM|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle = \lambda|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$$

for an eigenvalue λ independent of $i_1, \ldots, i_j$. Together with equation (12), this implies equation (10) with $a_{12} = \lambda/j$.

Equation (11) follows by proving

$$M^T|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle = c|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$$

and

$$CM^T|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle = \lambda|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle,$$

in a similar way.

We now diagonalize the matrix

$$M' = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}.$$

It has two eigenvectors: $\begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix}$ and $\begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix}$. Equation (9) implies that, for any $i_1, \ldots, i_j$,

$$\alpha_1|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle + \beta_1|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$$

is an eigenvector of M with the same eigenvalue λ. Therefore, $S_{\alpha_1,\beta_1,i}$ is an eigenspace of M. Similarly, $S_{\alpha_2,\beta_2,i}$ is an eigenspace of M. Vectors $\alpha_1|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle + \beta_1|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$ and $\alpha_2|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle + \beta_2|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$ together span the same space as vectors $|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$ and $|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$. Since vectors $|\tilde{\psi}^{i,l}_{i_1,\ldots,i_j}\rangle$ span $S^{i,l}_j$, this means that

$$S^{i,0}_j \cup S^{i,1}_j \subseteq S_{\alpha_1,\beta_1,i} \cup S_{\alpha_2,\beta_2,i}.$$

Therefore, repeating this argument for every i gives a collection of eigenspaces that span the entire state space for $\mathcal{H}_I$. This means that any eigenspace of M is a direct sum of some of eigenspaces $S_{\alpha,\beta,i}$. ■

Proof: [of Claim 11] For part (i), consider the states $|\psi_{i_1,\ldots,i_j}\rangle$ spanning T_j. We have

$$|\psi_{i_1,\ldots,i_j}\rangle = \sqrt{\frac{N-k}{N-j}}|\psi^{i,0}_{i_1,\ldots,i_j}\rangle + \sqrt{\frac{K-j}{N-j}}|\psi^{i,1}_{i_1,\ldots,i_j}\rangle \tag{14}$$

because a $\frac{N-K}{N-j}$ fraction of the states $|x_1 \ldots x_N\rangle$ with $|x| = K$ and $x_{i_1} = \ldots = x_{i_j} = 1$ have $x_i = 0$ and the rest have $x_i = 1$. The projection of these states to $(T^{i,0}_{j-1} \cup T^{i,1}_{j-1})^\perp$ are

$$\sqrt{\frac{N-K}{N-j}}|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle + \sqrt{\frac{K-j}{N-j}}|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$$

which, by equation (2) are exactly the states spanning $S^i_{\alpha_0,\beta_0,j}$. Furthermore, we claim that

$$T_{j-1} \subseteq T^{i,0}_{j-1} \cup T^{i,1}_{j-1} \subseteq T_j. \tag{15}$$

The first containment is true because T_{j-1} is spanned by the states $|\psi_{i_1,\ldots,i_{j-1}}\rangle$ which either belong to $T^{i,1}_{j-2} \subseteq T^{i,1}_{j-1}$ (if one of $i_1,\ldots,i_{j-1}$ is equal to i) or are a linear combination of states $|\psi^{i,0}_{i_1,\ldots,i_{j-1}}\rangle$ and $|\psi^{i,1}_{i_1,\ldots,i_{j-1}}\rangle$ which belong to $T^{i,0}_{j-1}$ and $T^{i,1}_{j-1}$. The second containment follows because the states $|\psi^{i,1}_{i_1,\ldots,i_{j-1}}\rangle$ spanning $T^{i,1}_{j-1}$ are the same as the states $|\psi_{i,i_1,\ldots,i_{j-1}}\rangle$ which belong to T_j and the states $|\psi^{i,0}_{i_1,\ldots,i_{j-1}}\rangle$ spanning $T^{i,0}_{j-1}$ can be expressed as linear combinations of $|\psi_{i_1,\ldots,i_{j-1}}\rangle$ and $|\psi_{i,i_1,\ldots,i_{j-1}}\rangle$ which both belong to T_j.

The first part of (15) now implies

$$S^i_{\alpha_0,\beta_0,j} \subseteq (T^{i,0}_{j-1} \cup T^{i,1}_{j-1})^\perp \subseteq (T_{j-1})^\perp.$$

We also have $S^i_{\alpha_0,\beta_0,j} \subseteq T_j$, because, $S^i_{\alpha_0,\beta_0,j}$ is spanned by the states

$$P_{(T^{i,0}_{j-1}\cup T^{i,1}_{j-1})^\perp}|\psi_{i_1,\ldots,i_j}\rangle = |\psi_{i_1,\ldots,i_j}\rangle - P_{T^{i,0}_{j-1}\cup T^{i,1}_{j-1}}|\psi_{i_1,\ldots,i_j}\rangle$$

and $|\psi_{i_1,\ldots,i_j}\rangle$ belongs to T_j by the definition of T_j and $P_{T^{i,0}_{j-1}\cup T^{i,1}_{j-1}}|\psi_{i_1,\ldots,i_j}\rangle$ belongs to T_j because of the second part of (15). Therefore, $S^i_{\alpha_0,\beta_0,j} \subseteq T_j \cap (T_{j-1})^\perp = S_j$.

For the part (ii), we have

$$S^i_{\alpha_0,\beta_0,j} \subseteq S^{i,0}_j \cup S^{i,1}_j \subseteq T^{i,0}_j \cup T^{i,1}_j \subseteq T_{j+1},$$

where the first containment is true because $S^i_{\alpha_0,\beta_0,j}$ is spanned by linear combinations of vectors $|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$ (which belong to $S^{i,0}_j$) and vectors $|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle$ (which belong to $S^{i,1}_j$) and the last containment is true because of the second part of equation (15).

Let

$$|\psi\rangle = \beta_0 \frac{|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle}{\||\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle\|} - \alpha_0 \frac{|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle}{\||\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle\|} \tag{16}$$

be one of the vectors spanning $S^i_{\beta_0,-\alpha_0,j}$. To prove that $|\psi\rangle$ is in $S_{j+1} = T_{j+1} - T_j$, it remains to prove that $|\psi\rangle$ is orthogonal to T_j. This is equivalent to proving that $|\psi\rangle$ is orthogonal to every of the vectors $|\psi_{i'_1,\ldots,i'_j}\rangle$ spanning T_j.

Case 1. $\{i'_1,\ldots,i'_j\} = \{i_1,\ldots,i_j\}$.

Since $|\psi\rangle$ belongs to $(T^{i,0}_{j-1} \cup T^{i,1}_{j-1})^\perp$, it suffices to prove that $|\psi\rangle$ is orthogonal to the projection of $|\psi_{i_1,\ldots,i_j}\rangle$ to $(T^{i,0}_{j-1} \cup T^{i,1}_{j-1})^\perp$ which, by discussion after the equation (14), is equal to

$$\alpha_0 \frac{|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle}{\||\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle\|} + \beta_0 \frac{|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle}{\||\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle\|}. \tag{17}$$

From equations (16) and (17), we see that the inner product of the two states is $\alpha_0\beta_0 - \beta_0\alpha_0 = 0$.

Case 2. $\{i'_1,\ldots,i'_j\} \neq \{i_1,\ldots,i_j\}$ but one of $i'_1,\ldots,i'_j$ is equal to i.

For simplicity, assume $i = i'_j$. Then, $|\psi_{i'_1,\ldots,i'_j}\rangle$ is the same as $|\psi^{i,1}_{i'_1,\ldots,i'_{j-1}}\rangle$ which belongs to $T^{i,1}_{j-1}$. By definition of $S^i_{\alpha,\beta,j}$, the vector $|\psi\rangle$ belongs to $(T^{i,0}_{j-1} \cup T^{i,1}_{j-1})^\perp$ and is therefore orthogonal to $|\psi^{i,1}_{i'_1,\ldots,i'_{j-1}}\rangle$.

Case 3. $\{i'_1,\ldots,i'_j\} \neq \{i_1,\ldots,i_j\}$ and none of $i'_1,\ldots,i'_j$ is equal to i.

One of $i'_1,\ldots,i'_j$ must be not in $\{i_1,\ldots,i_j\}$. For simplicity, assume it is i'_j. We have

$$|\psi_{i'_1,\ldots,i'_{j-1}}\rangle = \sum_{i' \notin \{i'_1,\ldots,i'_{j-1}\}} |\psi_{i'_1,\ldots,i'_{j-1},i'}\rangle.$$

Also, $\langle\psi_{i'_1,\ldots,i'_{j-1}}|\psi\rangle = 0$, because $|\psi_{i'_1,\ldots,i'_{j-1}}\rangle$ is in $T^{i,0}_{j-1} \cup T^{i,1}_{j-1}$. As proven in the previous case, $\langle\psi_{i'_1,\ldots,i'_{j-1},i}|\psi\rangle = 0$. We therefore have

$$\sum_{i' \notin \{i'_1,\ldots,i'_{j-1},i\}} \langle\psi_{i'_1,\ldots,i'_{j-1},i'}|\psi\rangle = 0. \tag{18}$$

By symmetry, the inner product $\langle\psi_{i'_1,\ldots,i'_{j-1},i'}|\psi\rangle$ is the same for every $i' \notin \{i'_1,\ldots,i'_{j-1},i\}$. Therefore, equation (18) means

$$\langle\psi_{i'_1,\ldots,i'_{j-1},i'}|\psi\rangle = 0$$

for every $i' \notin \{i'_1,\ldots,i'_{j-1},i\}$. ■

Proof: [of Claim 13] $\tau^i_{\alpha,\beta,j}$ is a mixture of states $|\psi\rangle$ from the subspace $S^i_{\alpha,\beta,j}$. We prove the claim by showing that, for any of those states $|\psi\rangle$, the squared norm of its projection to S_{j+1} is equal to the right hand side of claim 13. Since $|\psi\rangle \in S^i_{\alpha,\beta,j}$ we can write it as

$$|\psi\rangle = \sum_{i_1,\ldots,i_j} a_{i_1,\ldots,i_j}(\alpha|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle + \beta|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle)$$

for some $a_{i_1,\ldots,i_j}$. Let

$$|\psi^+\rangle = \sum_{i_1,\ldots,i_j} a_{i_1,\ldots,i_j}(\beta_0|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle - \alpha_0|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle),$$

$$|\psi^-\rangle = \sum_{i_1,\ldots,i_j} a_{i_1,\ldots,i_j}(\alpha_0|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle + \beta_0|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\rangle).$$

Then, $|\psi\rangle$ is a linear combination of $|\psi^+\rangle$ which belongs to $S^i_{\beta_0,-\alpha_0,j} \subset S_{j+1}$ (by Claim 11) and $|\psi^-\rangle$ which belongs to $S^i_{\alpha_0,\beta_0,j} \subseteq S_j$. Moreover, all three states are linear combinations of $|\psi^0\rangle$, $|\psi^1\rangle$ defined by

$$|\psi^l\rangle = \sum_{i_1,\ldots,i_j} a_{i_1,\ldots,i_j}|\tilde{\psi}^{i,l}_{i_1,\ldots,i_j}\rangle.$$

We have

$$|\psi\rangle = \alpha|\psi^0\rangle + \beta|\psi^1\rangle,$$

$$|\psi^+\rangle = \beta_0|\psi^0\rangle - \alpha_0|\psi^1\rangle,$$
$$|\psi^-\rangle = \alpha_0|\psi^0\rangle + \beta_0|\psi^1\rangle.$$

Since $|\psi^+\rangle$ and $|\psi^-\rangle$ belong to subspaces S_{j+1} and S_j which are orthogonal, we must have $\langle\psi^+|\psi^-\rangle = 0$. This means

$$\alpha_0\beta_0\|\psi^0\|^2 - \beta_0\alpha_0\|\psi^1\|^2 = 0.$$

By dividing the equation by $\alpha_0\beta_0$, we get $\|\psi^0\|^2 = \|\psi^1\|^2$ and $\|\psi^0\| = \|\psi^1\|$. Since $\|\psi\| = 1$, this means that $\|\psi^0\| = \|\psi^1\| = \frac{1}{\sqrt{\alpha^2+\beta^2}} = 1$.

Since $|\psi\rangle$ lies in the subspace spanned by $|\psi^+\rangle$ which belongs to S_{j+1} and $|\psi^-\rangle$ which belongs to S_j, the norm of the projection of $|\psi\rangle$ to S_{j+1} is equal to $\frac{|\langle\psi|\psi^+\rangle|}{\|\psi^+\|}$. By expressing $|\psi\rangle$, $|\psi^+\rangle$ in terms of $|\psi^0\rangle$, $|\psi^1\rangle$, we get

$$\frac{|\langle\psi|\psi^+\rangle|}{\|\psi^+\|} = \frac{\alpha\beta_0\|\psi^0\|^2 - \alpha_0\beta\|\psi^1\|^2}{\sqrt{\beta_0^2\|\psi^0\|^2 + \alpha_0^2\|\psi^0\|^2}} = \frac{|\alpha\beta_0 - \alpha_0\beta|}{\sqrt{\alpha_0^2+\beta_0^2}},$$

proving the claim. ■

Proof: [of Claim 14] We will prove $\|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\| \geq \frac{1}{2}\|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\|$, because that means

$$\alpha_0 = \frac{\sqrt{N-K}}{\sqrt{N-j}}\|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\| \geq \frac{1}{2}\frac{\sqrt{N-K}}{\sqrt{K-j}}\frac{\sqrt{K-j}}{\sqrt{N-j}}\|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\| = \frac{\sqrt{N-K}}{2\sqrt{K-j}}\beta_0$$

and

$$\frac{\beta_0}{\sqrt{\alpha_0^2+\beta_0^2}} \leq \frac{\beta_0}{\sqrt{\frac{N-K}{4(K-j)}\beta_0^2 + \beta_0^2}} = \frac{1}{\sqrt{1+\frac{N-K}{4(K-j)}}} = \frac{\sqrt{4(K-j)}}{\sqrt{N+3K-4j}}.$$

To prove $\|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\| \geq \|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\|$, we calculate the vector

$$|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle = P_{(T^{i,0}_{j-1})^\perp}|\psi^{i,0}_{i_1,\ldots,i_j}\rangle.$$

Both vector $|\psi^{i,0}_{i_1,\ldots,i_j}\rangle$ and subspace $T^{i,0}_{j-1}$ are fixed by

$$U_\pi|x\rangle = |x_{\pi(1)}\ldots x_{\pi(N)}\rangle$$

for any permutation π that fixes i and maps $\{i_1,\ldots,i_j\}$ to itself. This means that $|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$ is fixed by any such U_π as well. Therefore, the amplitude of $|x\rangle$, $|x| = K$, $x_i = 0$ in $|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$ only depends on $|\{i_1,\ldots,i_j\}\cap\{t : x_t = 1\}|$. This means $|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$ is of the form

$$|\psi_0\rangle = \sum_{m=0}^{j}\alpha_m \sum_{\substack{x:|x|=K,x_i=0\\ |\{i_1,\ldots,i_j\}\cap\{t:x_t=1\}|=m}} |x\rangle.$$

To simplify the following calculations, we multiply α_0, …, α_j by the same constant so that $\alpha_j = 1/\sqrt{\binom{N-j-1}{K-j}}$. Then, $|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle$ remains a multiple of $|\psi_0\rangle$ but may no longer be equal to $|\psi_0\rangle$.

$\alpha_0, \ldots, \alpha_{j-1}$ should be such that the state is orthogonal to T_{j-1} and, in particular, orthogonal to states $|\psi^{i,0}_{i_1,\ldots,i_l}\rangle$ for $l \in \{0,\ldots,j-1\}$. By writing out $\langle\psi_0|\psi^{i,0}_{i_1,\ldots,i_l}\rangle = 0$, we get

$$\sum_{m=l}^{j} \alpha_m \binom{N-j-1}{K-m}\binom{j-l}{m-l} = 0. \tag{19}$$

To show that, we first note that $|\psi^{i,0}_{i_1,\ldots,i_l}\rangle$ is a uniform superposition of all $|x\rangle$, $|x| = K$, $x_i = 0$, $x_{i_1} = \ldots = x_{i_l} = 1$. If we want to choose x subject to those constraints and also satisfying $|\{i_1,\ldots,i_j\} \cap \{t : x_t = 1\}| = m$, we have to set $x_t = 1$ for $m-l$ different $t \in \{i_{l+1},\ldots,i_j\}$ and for $K-m$ different $t \notin \{i, i_1,\ldots,i_j\}$. This can be done in $\binom{j-l}{m-l}$ and $\binom{N-j-1}{K-m}$ different ways, respectively.

By solving the system of equations (19), we get that the only solution is

$$\alpha_m = (-1)^{j-m}\frac{\binom{N-j-1}{K-j}}{\binom{N-j-1}{K-m}}\alpha_j. \tag{20}$$

Let $|\psi'_0\rangle = \frac{|\psi_0\rangle}{\|\psi_0\|}$ be the normalized version of $|\psi_0\rangle$. Then,

$$|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\rangle = \langle\psi'_0|\psi^{i,0}_{i_1,\ldots,i_j}\rangle|\psi'_0\rangle,$$

$$\|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\| = \langle\psi'_0|\psi^{i,0}_{i_1,\ldots,i_j}\rangle = \frac{\langle\psi_0|\psi^{i,0}_{i_1,\ldots,i_j}\rangle}{\|\psi_0\|} \tag{21}$$

First, we have

$$\langle\psi_0|\psi^{i,0}_{i_1,\ldots,i_j}\rangle = 1,$$

because $|\psi^{i,0}_{i_1,\ldots,i_j}\rangle$ consists of $\binom{N-j-1}{K-j}$ basis states $|x\rangle$, $x_i = 0$, $x_{i_1} = \ldots = x_{i_j} = 1$, each of which has amplitude $1/\sqrt{\binom{N-j-1}{K-j}}$ in both $|\psi_0\rangle$ and $|\psi^{i,0}_{i_1,\ldots,i_j}\rangle$. Second,

$$\|\psi_0\|^2 = \sum_{m=0}^{j}\binom{j}{m}\binom{N-j-1}{K-m}\alpha_m^2 = \sum_{m=0}^{j}\binom{j}{m}\frac{\binom{N-j-1}{K-j}^2}{\binom{N-j-1}{K-m}}\alpha_j^2$$

$$= \sum_{m=0}^{j}\binom{j}{m}\frac{\binom{N-j-1}{K-j}}{\binom{N-j-1}{K-m}} = \sum_{m=0}^{j}\binom{j}{m}\frac{(K-m)!(N-K+m-j-1)!}{(K-j)!(N-K-1)!}$$

$$= \sum_{m=0}^{j}\binom{j}{m}\frac{(K-m)\ldots(K-j+1)}{(N-K-1)\ldots(N-K+m-j)} \tag{22}$$

with the first equality following because there are $\binom{j}{m}\binom{N-j-1}{K-m}$ vectors x such that $|x| = K$, $x_i = 0$, $x_t = 1$ for m different $t \in \{i_1,\ldots,i_j\}$ and $K-m$ different $t \notin \{i, i_1,\ldots,i_j\}$, the second equality following from equation (20) and the third equality following from our choice $\alpha_j = 1/\sqrt{\binom{N-j-1}{K-j}}$.

We can similarly calculate $\|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\|$. We omit the details and just state the result. The counterpart of equation (21) is

$$\|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\| = \frac{\langle\psi_1|\psi^{i,1}_{i_1,\ldots,i_j}\rangle}{\|\psi_1\|},$$

with $|\psi_1\rangle$ being the counterpart of $|\psi_0\rangle$:

$$|\psi_1\rangle = \sum_{m=0}^{j} \alpha_m \sum_{\substack{x:|x|=K,x_i=1 \\ |\{i_1,\ldots,i_j\}\cap\{l:x_l=1\}|=m}} |x\rangle,$$

with $\alpha_0 = 1/\sqrt{\binom{N-j-1}{K-j-1}}$. Similarly as before, we get $\langle\psi_1|\psi^{i,1}_{i_1,\ldots,i_j}\rangle = 1$ and

$$\|\psi_1\|^2 = \sum_{m=0}^{j} \binom{j}{m} \frac{\binom{N-j-1}{K-j-1}}{\binom{N-j-1}{K-m-1}}$$

$$= \sum_{m=0}^{j} \binom{j}{m} \frac{(K-m-1)\ldots(K-j)}{(N-K)\ldots(N-K+m-j+1)} \tag{23}$$

Each term in (22) is $\frac{(K-m)(N-K+m-j)}{(K-j)(N-K)}$ times the corresponding term in equation (23). We have

$$\frac{K-m}{K-j}\frac{N-K+m-j}{N-K} \leq \frac{K}{K/2}\cdot 2 = 4,$$

because $j \leq K/2$ and $N-K+m-j \leq N-K$ (because of $m \leq j$). Therefore, $\|\psi_0\|^2 \leq 4\|\psi_1\|^2$ which implies

$$\|\tilde{\psi}^{i,0}_{i_1,\ldots,i_j}\| = \frac{1}{\|\psi_0\|} \geq \frac{1}{\sqrt{4}\|\psi_1\|} = \frac{1}{2}\|\tilde{\psi}^{i,1}_{i_1,\ldots,i_j}\|.$$

■

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